Quantum fluctuation driven first order phase transition in weak ferromagnetic metals

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In a local Fermi liquid (LFL), we show that there is a line of weak first order phase transitions between the ferromagnetic and paramagnetic phases due to purely quantum fluctuations. We predict that an instability towards superconductivity is only possible in the ferromagnetic state. At $T = 0$ we find a point on the phase diagram where all three phases meet and we call this a quantum triple point (QTP). A simple application of the Gibbs phase rule shows that only these three phases can meet at the QTP. This provides a natural explanation of the absence of superconductivity at this point coming from the paramagnetic side of the phase diagram, as observed in the recently discovered ferromagnetic superconductor, UGe_2.

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The study of weak itinerant ferromagnetism, both experimentally and theoretically, is an extremely important topic in understanding strongly correlated electron systems. It has been shown over the past five years or so that materials which can be considered weak ferromagnets (small Curie temperature) display a very wide assortment of complex phenomena and novel physical properties. For example, UGe_2, $ZrZn_2$, and $URhGe$ have been observed to be superconducting *and* ferromagnetic, whereas it had previously been expected (yet not observed) to be superconducting on only the paramagnetic side of the phase transition [1, 2, 3]. It is even more interesting because this superconductivity might be BCS-like, i.e., singlet pairing, as opposed to all of the recent models which predict triplet pairing. The s-wave singlet model has been considered by these authors and others and there are no definite answers as of yet [4, 5, 6, 7, 8]. A new result reported recently [9] shows that the magnetic transitions in the heavy fermion itinerant ferromagnetic superconductor UGe_2 are of first order, and therefore there does not exist a quantum critical point as previously thought.

In this Letter we propose an explanation of the observed first order magnetic transition and superconducting behavior based on the 'Induced Interaction Model' first proposed by Babu and Brown [10] *and* the general properties of a Local Fermi Liquid. As explained below, this analysis leads to a thermodynamically consistent, first order phase transition from the ferromagnetic state to the paramagnetic state. We end by considering some aspects of the superconductivity.

The local Fermi liquid (LFL) was a concept proposed by Engelbrecht and Bedell to look at normal paramagnetic metals [11]. It is a generalization of the LFL proposed by Nozières while studying the single impurity Kondo problem [12]. Blagoev *et al* recently studied a LFL to explain weak ferromagnetic metals [5, 6]. This was shown to reproduce non-trivial results and even the possibility of superconductivity. The superconductivity was predicted to be s-wave on the ferromagnetic side, due to the constraint of the LFL, and it had been speculated to be p-wave on the paramagnetic side. While the nature of the superconducting order parameter is still in question, the real mystery is why superconductivity is only found in the ferromagnetic state.

To gain insight into this problem, we start with a simple model that can describe a strongly correlated Fermi liquid, the LFL of ref.[11]. This theory makes the assumption that the quasiparticle self-energy $\Sigma(\omega)$ is momentum independent. This leads to a further simplification in the theory since only the s-wave Fermi liquid parameters and scattering amplitudes are nonzero. In the limit of small magnetic moment, the scattering amplitude in the LFL can be expressed as $A_0^{\sigma\sigma'} = A_0^s + A_0^a \sigma \cdot \sigma'$, where the $A's$ are the scattering amplitudes, related to the Landau parameters by $A_0^{s,a} = F_0^{s,a}/(1 + F_0^{s,a})$. Note that here and elsewhere, the capital letter quantities have been made dimensionless by multiplication by the density of states, $A = N(0)a$ and $F = N(0)f$. In the LFL the forward scattering sum rule, which is a consequence of the Pauli principle, imposes the constraint that $A_0^{\uparrow\uparrow} = A_0^s + A_0^a = 0$. It can be shown that when these constraints are applied to a paramagnetic Fermi liquid, the system is stable against a transition to a ferromagnetic state and also against phase separation [11], i.e., as ${F_0}^s$ gets large then ${F_0}^a$ saturates to -$\frac{1}{2}$ and superconductivity in both the s and p-wave channels is suppressed.

These results change dramatically when the LFL is applied to a weak ferromagnetic system (see refs.[5, 6] for more details). In the vicinity of the phase transition, ${F_0}^a \to -1^-$ and ${F_0}^s \to -1^+$ and both scattering amplitudes diverge, indicating an instability in the spin (${A_0}^a$) and in the charge (${A_0}^s$) sector. The ferromagnetism remains while the singlet scattering amplitude, A_0^{sing}, is attractive. This opens up the possibility of the existence of s-wave superconductivity since the triplet scattering amplitude is strictly zero in the LFL.

For small magnetization and low temperatures and energies, one can see that this description remains valid within weak ferromagnetic Fermi liquid theory. However,

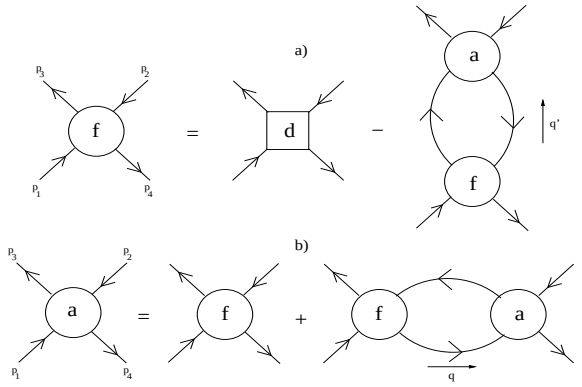

FIG. 1: The schematic integral equations for the Landau f-function and the scattering amplitudes a. The $\vec{p}$'s are the incoming and outgoing particle momenta. Note how the interaction in a) is graphically shown to be decomposed into a direct term d and the induced term. Part b) is the fully reducible set of diagrams.

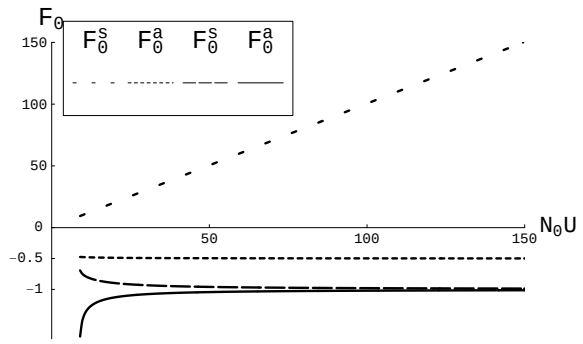

FIG. 2: The two sets of solutions for the paramagnetic state (top two lines) and the ferromagnetic state (bottom two lines). The limiting values for large $N(0)U$ of $F_0^{a,s}$ are given in the text. Please note the change in scale of the y-axis shown for clarity.

as m_0 (magnetization) gets even smaller as one moves toward the critical transition, the situation changes. Since in the local limit, $m^*/m \sim z^{-1} \sim \log m_0$, around the critical point the effective mass diverges, the quasiparticle residue z goes to zero, and the validity of Fermi liquid theory becomes questionable. Hence, the ferromagnetic and paramagnetic LFL states are not *continuously* connected through the critical point within this theory. But, and this is a crucial point, if the transition is 'preempted' by a first-order transition as to restrict or limit the divergences, then we can recover a consistent theory. This is indeed what is seen to happen as will be explained below.

We have shown that the LFL yields unexpected and quite distinct predictions about the behavior of the paramagnetic and ferromagnetic Fermi liquids. Moreover, we argued that they are not connected by a continuous second order phase transition. What we will show here is that they are in fact connected by a first order transition using the 'Induced Interaction Model' [10], which was further developed by Bedell and collaborators [13, 14]. This a model for self-consistently calculating the quasiparticle scattering amplitude (fully reducible interaction) in terms of the three interaction channels: particle-hole, exchange particle-hole(induced interaction), and the particle-particle channel.

Including all three channels gives rise to a properly antisymmetrized scattering amplitude, a, where $N(0)a = A$. The diagrammatic structure of these equations is shown in Fig.1. The direct interaction, d, is an antisymmetrized effective two-body potential in the particle-particle channel. It is chosen specifically for a certain physical model, i.e., it contains information about the underlying Hamiltonian. The second set of diagrams on the right side of Fig.1a) is the exchange of topologically equivalent diagrams in Fig.1b). Thus, the induced interaction is a purely quantum effect, arising from the exchange diagrams that are required to antisymmetrize the effective two-body scattering amplitude.

To determine the Fermi liquid parameters, we study the equations of Fig.1 in the limit of the momentum transfer, $\vec{q} = \vec{p_1} - \vec{p_3} = 0$ [13, 14]. In the local limit of these equations, the induced interactions are equivalent to the limit of the exchange momentum transfer $\vec{q'} = \vec{p_1} - \vec{p_4} = 0$. The full momentum dependence of the interactions on the Fermi surface has been investigated extensively in the paramagnetic phase [13, 14], and we are currently extending this approach to the ferromagnetic phase [15]. Including the full momentum dependence will not change the results we describe here in any qualitative way. Thus for our purposes, we will focus here on the local limit of the model to calculate the quasiparticle interactions for both the ferromagnetic and paramagnetic LFL. In the local limit, the coupled *integral* equations [13, 14] of Fig.1a) and 1b) reduce to two coupled *algebraic* equations,

$$F_0^s = D_0^s + \frac{1}{2}F_0^s A_0^s + \frac{3}{2}F_0^a A_0^a \tag{1}$$

$$F_0^a = D_0^a + \frac{1}{2}F_0^s A_0^s - \frac{1}{2}F_0^a A_0^a. \tag{2}$$

The LFL picture, now coupled with the induced interaction model, gives a description of a weak ferromagnetic Fermi liquid and its *first order* transition to the paramagnetic Fermi liquid. We will take the antisymmetrized direct interaction to be $D_0^s = -D_0^a = N(0)U/2$, where U is the 'on-site' contact interaction, such as in the Hubbard model. This is our model-dependent parameter.

We solve eqtn's (1,2) self-consistently using the above form of the direct interaction. We show the results graphically in Fig.2. The different branches for each solution are described in the caption. The important consequence is that in the large $N(0)U$ limit, the solutions remarkably yield exactly the same results as those of the LFL,

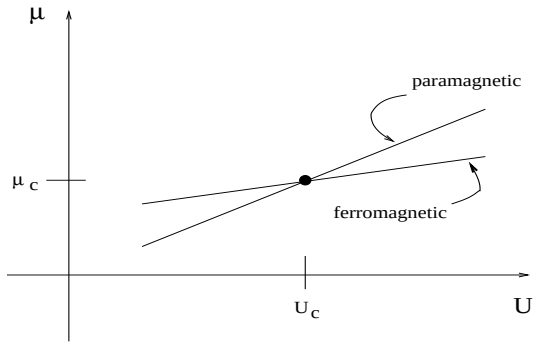

FIG. 3: The shape of the chemical potential curves expanded around the critical U_c. Note how the higher U regime is the one in which the ferromagnetic state has the lower energy.

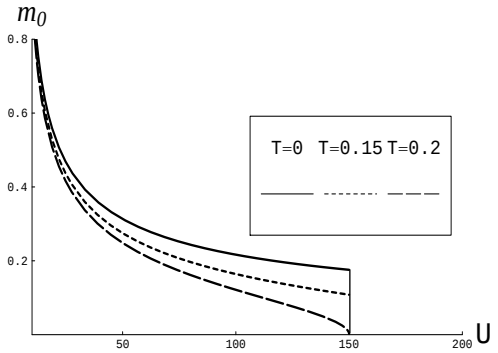

FIG. 4: The equilibrium magnetization plotted as a function of the effective interaction $\bar{U} = N(0)U$ for different T. The temperatures in this model are scaled by the spin fluctuation temperature, which is about 1/100 of the Fermi temperature for the interaction strengths of interest. The moment drops discontinuously to zero at the critical $\bar{U}_c = 150$ at zero temperature and for $T < T_c$ (shown by the vertical line), yet continuously to zero at the critical temperature $T_c = 0.2$, indicating a crossover from first order to second order. See Fig.5.

namely, $F_0^s \to \infty$ and $F_0^a \to -1/2$ in one case, and $F_0^s \to -1^+$ and $F_0^a \to -1^-$ in the other.

Investigating the model more closely we will now employ certain aspects of a spin-polarized Fermi liquid to the thermodynamics of the system. In this theory the Landau parameters are modified due to a finite magnetization in the ferromagnetic state. For full details see [16, 17] and references therein. This has consequences for the effective masses m_σ^* of each spin species, as well as for the Fermi momenta k_F^σ of each Fermi surface, since the magnetization dependence of these quantities is extremely important.

Since the multiple solutions of this model are found for every U at large enough U, one can imagine the system, for some specific U, jumping from one solution to the other (see Fig.2). This can be shown by examining the chemical potential as a function of U. We can expand the chemical potential around a certain U_c which determines where one state gives way to another state of lower energy. The point at which the chemical potentials cross is the point of the first order phase transition. To see this, we calculate the change in the chemical potential due to the change in the magnetization for fixed density, n, which is given by $\delta\mu = \frac{1}{4}(C^{\uparrow\uparrow} - C^{\downarrow\downarrow})\delta m$, where $C^{\sigma\sigma} = 1/N^\sigma(0) + \tilde{f}_0^{\ \sigma\sigma}$ and $N_0^\sigma(0) = k_F^\sigma m_\sigma^*/2\pi^2$ is the density of states at the Fermi surface of spin σ (the tilde distinguishes the Landau parameters in the polarized state). Then the chemical potentials for the two phases near U_c are written as follows:

$$\mu_F(U) \approx \mu_c(U_c) + (U - U_c)\frac{d\mu_F(U = U_c)}{dU} \qquad (3)$$

$$\mu_P(U) \approx \mu_c(U_c) + (U - U_c)\frac{d\mu_P(U = U_c)}{dU}. \qquad (4)$$

We differentiate the chemical potential in the ferromagnetic state implicitly through the magnetization which is itself a function of U. This is seen, for example, through the relation for the equilibrium magnetization in a weak ferromagnet: $m_0 \sim |1 + F_0^a(U)|^\alpha$, where α depends on the order in which the Ginzburg-Landau type expansion is carried to in the magnetization ($\alpha = 1/2$ for maximal m^4 term, 1/4 for m^6, etc.). This holds for small m_0 [5]. It is seen in Fig.3 that for smaller U the paramagnetic state is favored but at the critical value U_c the chemical potentials cross and the ferromagnetic state is the lower energy state.

Extending these calculations to low but finite temperatures can be done using certain thermodynamic Maxwell relations. Doing this we can map out the temperature phase diagram. The concern will be with the chemical potential and the pressure at finite temperatures and small magnetizations where we apply the same analysis we did at zero temperature. The details will be shown elsewhere, but the first step is to integrate the Maxwell relation, $-\left(\frac{\partial s}{\partial n}\right)_{T,m} = \left(\frac{\partial \mu}{\partial T}\right)_{n,m}$, with respect to T, where the entropy density s is given by the usual low temperature Fermi liquid approximation $s(n, m, T) = \gamma(n, m)T$ [16]. This results in a magnetization-dependent chemical potential expansion in m and up to second order in T. A similar method is used to develop a free energy expansion in the magnetization and the temperature. By differentiation of the free energy, an expression for the temperature-dependent magnetization can be derived. And finally the pressure, $P = -f + \mu n + Hm$, can be calculated from the free energy to give an expression in terms of small magnetization and low temperatures:

$$P(m, T) = P(0, 0) + N_0\frac{\pi^2}{6}T^2 - n\frac{\partial N_0}{\partial n}\frac{\pi^2}{6}T^2$$
$$+G_1 m^2 + G_2 m^4 + G_3 m^2\frac{\pi^2}{6}T^2 + G_4 m^4\frac{\pi^2}{6}T^2. \qquad (5)$$

The coefficients G_i depend on the Landau interaction

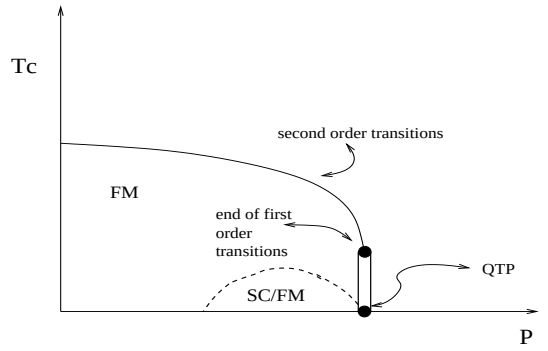

FIG. 5: The T_c versus P schematic phase diagram generated from this model. The double line indicates the line of first order transitions, which ends at a finite T, estimated in the text below. The SC dome, calculated from LFL theory only, is taken from ref's [5, 6]. The superconducting transition at low temperatures near the QTP is still under investigation as to its order. For further discussion on this point, see [18].

functions and the polarization expansion coefficients of quantities such as the effective mass [15].

Now we can determine what happens at temperatures away from zero. At zero temperature the magnetization jumps discontinuously to zero at a certain U indicating a first order transition. However, as shown in Fig.4, when the temperature is turned on, we see that for a certain critical $\bar{U}_c$, and above a certain temperature $T_c \neq 0$, the magnetization goes continuously to zero, indicating a second order transition. This implies that there is a line of first order transitions that ends and soon becomes a line of second order transitions at finite temperatures.

To 'translate' from U back to a physical control parameter, such as pressure, we take advantage of the thermodynamics described above to develop the phase diagram. The results are shown in Fig.5. The steep slope of the transition near the critical pressure is due to the fact that the latent heat of the transition, which is zero at $T = 0$, is also zero or nearly zero at small temperatures. This is because the entropy difference between the FM and PM states is proportional to the DOS difference on each side, which to leading order is zero, and to the next higher order is $O(m^2)$, where m is small. Thus these transitions are truly weakly first order. What we see strikingly resembles the experimental phase diagram of UGe_2. Looking at the physical values of this system, our effective chosen $\bar{U}_c = 150$. An approximate calculation of the DOS of UGe_2 at the Fermi surface yields a value of $\approx 20/eV$ [19]. This puts U in a range of $10eV$, a typical value for correlated electron systems. Our scaled $T_c = 0.2$ gives, when a typical Fermi temperature of $1 - 10eV$ is used, a critical temperature of around $1meV$, or about $10K$, the same order of magnitude as seen in the crossover regime of UGe_2.

One final thermodynamical observation can be made when looking at what we call the quantum triple point, QTP. At this point, as is shown in Fig.5, three phases end at zero temperature. According to the Gibbs phase rule [20], a single component system, which we have here, can only accomodate a maximum of three phases coexisting at a point. This restrictive condition explains why superconductivity can only be observed on *one* side of the QTP, and, as shown in previous studies [5, 6], this must be the ferromagnetic side, where consequently only pairing in the singlet channel is attractive. This is seen experimentally.

In summary, we explicitly have here a microscopic model that unmistakably yields a first order phase transition from the ferromagnetic to the paramagnetic state by the inclusion of the *quantum* fluctuations that arise from the induced interactions. This can be considered the quantum analogue to the case of first order transitions driven by *classical* fluctuations in certain liquid crystals studied by Brazovskii [21]. Consequently, if we turn off the (quantum) induced terms in our picture, the model reduces to a Stoner model which is just a standard second order transition between the ferromagnetic and paramagnetic phases. We show that the superconductivity is s-wave and only exists in the ferromagnetic state, and that, as a consequence of the Gibbs phase rule, there are only three phases that meet precisely at the quantum triple point.

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